1,2-Cyclohexanedicarboxylic acid, cyclohex-3-enylmethyl nonyl ester

Inchi: InChI=1S/C24H40O4/c1-2-3-4-5-6-7-13-18-27-23(25)21-16-11-12-17-22(21)24(26)28-19

InchiKey: WGHFEGCTVHDRSB-UHFFFAOYSA-N

Formula: C24H40O4

SMILES: CCCCCCCCCOC(=O)C1CCCCC1C(=O)OCC1CC=CCC1

Mol. weight [g/mol]: 392.57

Physical Properties

Property code	Value	Unit	Source
gf	-245.49	kJ/mol	Joback Method
hf	-882.21	kJ/mol	Joback Method
hfus	49.45	kJ/mol	Joback Method
hvap	88.17	kJ/mol	Joback Method
log10ws	-6.51		Crippen Method
logp	5.986		Crippen Method
mcvol	337.880	ml/mol	McGowan Method
pc	1098.62	kPa	Joback Method
rinpol	2817.00		NIST Webbook
rinpol	2817.00		NIST Webbook
tb	934.69	K	Joback Method
tc	1150.40	K	Joback Method
tf	515.84	K	Joback Method
vc	1.278	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1185.27	J/mol×K	934.69	Joback Method
cpg	1204.06	J/mol×K	970.64	Joback Method
cpg	1221.04	J/mol×K	1006.59	Joback Method
cpg	1236.23	J/mol×K	1042.55	Joback Method
cpg	1249.69	J/mol×K	1078.50	Joback Method
cpg	1261.45	J/mol×K	1114.45	Joback Method
cpg	1271.55	J/mol×K	1150.40	Joback Method
dvisc	0.0007306	Pa×s	515.84	Joback Method

dvisc	0.0003478	Pa×s	585.65	Joback Method
dvisc	0.0001939	Pa×s	655.46	Joback Method
dvisc	0.0001210	Pa×s	725.26	Joback Method
dvisc	0.0000820	Pa×s	795.07	Joback Method
dvisc	0.0000592	Pa×s	864.88	Joback Method
dvisc	0.0000449	Pa×s	934.69	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339872&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume